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NEWS Web Page URLs for STN Seminar Schedule - N. America NEWS Sep 17 IMSworld Pharmaceutical Company Directory name change to PHARMASEARCH NEWS 3 Oct 09 Korean abstracts now included in Derwent World Patents Index Oct 09 NEWS Number of Derwent World Patents Index updates increased Oct 15 NEWS Calculated properties now in the REGISTRY/ZREGISTRY File NEWS 6 Oct 22 Over 1 million reactions added to CASREACT NEWS 7 Oct 22 DGENE GETSIM has been improved NEWS 8 Oct 29 AAASD no longer available NEWS 9 Nov 19 New Search Capabilities USPATFULL and USPAT2 NEWS 10 Nov 19 TOXCENTER(SM) - new toxicology file now available on STN NEWS 11 Nov 29 COPPERLIT now available on STN NEWS 12 Nov 29 DWPI revisions to NTIS and US Provisional Numbers NEWS 13 Nov 30 Files VETU and VETB to have open access NEWS 14 Dec 10 WPINDEX/WPIDS/WPIX New and Revised Manual Codes for 2002 NEWS 15 Dec 10 DGENE BLAST Homology Search NEWS 16 Dec 17 WELDASEARCH now available on STN NEWS 17 Dec 17 STANDARDS now available on STN NEWS 18 Dec 17 New fields for DPCI NEWS 19 Dec 19 CAS Roles modified NEWS 20 Dec 19 1907-1946 data and page images added to CA and CAplus NEWS 21 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web NEWS 22 Jan 25 Searching with the P indicator for Preparations NEWS 23 Jan 29 FSTA has been reloaded and moves to weekly updates

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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NEWS 24

Feb 01

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TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

```
=> s fisetin/cn
L1
             1 FISETIN/CN
=> d
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
L1
RN
     528-48-3 REGISTRY
CN
     4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,7-dihydroxy- (9CI) (CA
     INDEX NAME)
OTHER CA INDEX NAMES:
CN
     Fisetin (6CI)
CN
     Flavone, 3,3',4',7-tetrahydroxy- (8CI)
OTHER NAMES:
CN
     3,3',4',7-Tetrahydroxyflavone
CN
     5-Desoxyquercetin
     Bois Bleu de Hongrie
CN
CN
     C.I. 75620
     C.I. Natural Brown 1
CN
CN
     Cotinin
CN
     Fiestin
```

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Fustel
CN
CN
     Fustet
     Junger Fustik
CN
CN
     Superfustel
     Superfustel K
CN
CN
     Ungarisches Gelbholz
     Ventin Sumach
CN
     Viset
CN
CN
     Young Fustic
     Young Fustic Crystals
CN
     Zante Fustic
CN
FS
     3D CONCORD
MF
     C15 H10 06
CI
     COM
LC
     STN Files:
```

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, HODOC*, IPA, MEDLINE, MRCK*, NAPRALERT, NIOSHTIC, PIRA, PROMT, RTECS*, TOXCENTER, TOXLIT, USPATFULL, VETU

(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

562 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
563 REFERENCES IN FILE CAPLUS (1967 TO DATE)
39 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> sel name E1 THROUGH E21 ASSIGNED

=> fil capl COST IN U.S. DOLLARS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
6.17
6.32

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FILE COVERS 1907 - 9 Feb 2002 VOL 136 ISS 7 FILE LAST UPDATED: 7 Feb 2002 (20020207/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

```
=> s l1 or fisetin
           565 L1
           516 FISETIN
             3 FISETINS
           519 FISETIN
                  (FISETIN OR FISETINS)
L2
           684 L1 OR FISETIN
=> s cellul? or ?obes? or weight loss or weight reduc? or lipoly?
        576009 CELLUL?
        123450 ?OBES?
         84518 WEIGHT
          7488 WEIGHTS
         89900 WEIGHT
                  (WEIGHT OR WEIGHTS)
       1245811 WT
         92979 WTS
       1293861 WT
                  (WT OR WTS)
       1319171 WEIGHT
                  (WEIGHT OR WT)
        462312 LOSS
         90953 LOSSES
        523939 LOSS
                  (LOSS OR LOSSES)
         38378 WEIGHT LOSS
                  (WEIGHT (W) LOSS)
         84518 WEIGHT
          7488 WEIGHTS
         89900 WEIGHT
                  (WEIGHT OR WEIGHTS)
       1245811 WT
         92979 WTS
       1293861 WT
                  (WT OR WTS)
       1319171 WEIGHT
                  (WEIGHT OR WT)
       1616067 REDUC?
        716238 REDN
```

1

```
37510 REDNS
        739655 REDN
                 (REDN OR REDNS)
       2029523 REDUC?
                 (REDUC? OR REDN)
          3306 WEIGHT REDUC?
                 (WEIGHT (W) REDUC?)
         15755 LIPOLY?
        746419 CELLUL? OR ?OBES? OR WEIGHT LOSS OR WEIGHT REDUC? OR LIPOLY?
1.3
=> s 12 (s) 13
            10 L2 (S) L3
=> d 1-5
L4
     ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS
AN
     1999:147371 CAPLUS
DN
     130:218273
TΙ
     Phosphotyrosine phosphatase inhibitors or tyrosine kinase activators for
     controlling cellular proliferation
IN
     Schieven, Gary L.
PA
     Bristol-Myers Squibb Company, USA
     U.S., 73 pp., Cont.-in-part of U.S. Ser. No. 189,330.
SO
     CODEN: USXXAM
DT
     Patent
LΑ
     English
FAN.CNT 2
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
     -----
                            -----
PΤ
     US 5877210
                      Α
                            19990302
                                           US 1995-465813
                                                          19950605
     US 5565491
                      Α
                            19961015
                                           US 1994-189330
                                                            19940131
                      AA
     CA 2179715
                            19950803
                                           CA 1995-2179715 19950130
     US 5583242
                      Α
                            19961210
                                           US 1995-450342
                                                            19950525
     US 5693627
                            19971202
                                           US 1995-450401
                      Α
                                                            19950525
PRAI US 1994-189330
                            19940131
RE.CNT 19
              THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS
L4
AN
     1995:258964 CAPLUS
DN
     122:75763
     Interplay between excited-state intramolecular proton transfer and charge
ΥТ
     transfer in flavonols and their use as protein-binding-site fluorescence
     probes
     Sytnik, Alexander; Gormin, David; Kasha, Michael
ΑU
     Inst. Mol. Biophys. Dep. Chem., Florida State Univ., Tallahassee, FL,
CS
     32306-3015, USA
     Proc. Natl. Acad. Sci. U. S. A. (1994), 91(25), 11968-72
SO
     CODEN: PNASA6; ISSN: 0027-8424
DT
     Journal
     English
LA
L4
     ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS
AN
     1994:208331 CAPLUS
DN
     120:208331
ΤI
     Potentiation of .beta.-adrenoceptor agonist-mediated lipolysis
     by quercetin and fisetin in isolated rat adipocytes
ΑU
     Kuppusamy, U. R.; Das. N. P.
     Fac. Med., Natl. Univ. Singapore, Singapore, 0511, Singapore
CS
SO
     Biochem. Pharmacol. (1994), 47(3), 521-9
     CODEN: BCPCA6; ISSN: 0006-2952
```

```
DT
     Journal
     English
LΑ
     ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS
T.4
AN
     1993:225097 CAPLUS
     118:225097
DN
     Ascorbic acid-enhanced antiproliferative effect of flavonoids on squamous
TI
     cell carcinoma in vitro
ΑU
     Kandaswami, Chithan; Perkins, Eddie; Soloniuk, Donald S.; Drzewiecki,
     Gary; Middleton, Elliott, Jr.
     Sch. Med. Biomed. Sci., State Univ. New York, Buffalo, NY, 14203, USA
CS
     Anti-Cancer Drugs (1993), 4(1), 91-6
SO
     CODEN: ANTDEV; ISSN: 0959-4973
DT
     Journal
     English
LA
     ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS
L4
     1992:625763 CAPLUS
AN
     117:225763
DN
TI
     Effects of flavonoids on cyclic AMP phosphodiesterase and lipid
     mobilization in rat adipocytes
ΑU
     Kuppusamy, U. R.; Das, N. P.
     Fac. Med., Natl. Univ. Singapore, Singapore, 0511, Singapore
CS
     Biochem. Pharmacol. (1992), 44(7), 1307-15
SO
     CODEN: BCPCA6; ISSN: 0006-2952
DT
     Journal
     English
LΑ
=> d ibib abs kwic 3, 5
     ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER:
                         1994:208331 CAPLUS
DOCUMENT NUMBER:
                          120:208331
TITLE:
                          Potentiation of .beta.-adrenoceptor agonist-mediated
                          lipolysis by quercetin and fisetin
                          in isolated rat adipocytes
AUTHOR (S):
                          Kuppusamy, U. R.; Das. N. P.
CORPORATE SOURCE:
                          Fac. Med., Natl. Univ. Singapore, Singapore, 0511,
                          Singapore
SOURCE:
                          Biochem. Pharmacol. (1994), 47(3), 521-9
                          CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE:
                          Journal
LANGUAGE:
                          English
     Quercetin and fisetin, two naturally occurring bioflavonoids mobilized
     lipids and enzymes in the absence or presence of epinephrine in intact rat
     adipocytes. Dose-(0-250 .mu.M) and time-(0-2 h) course studies, showed
     that they stimulated phosphodiesterase (PDE) activity and simultaneously
     exert cAMP accumulation. These bioflavonoids when present either singly
     or together with epinephrine stimulated the membrane-bound PDE but not the
     cytosolic PDE. The stimulation may act as a feedback mechanism to
     terminate the cAMP effects. The action of theophylline, a known
     lipolytic agent (exerting its effects through antagonism of
     adenosine Al receptor as well as PDE inhibition) was not potentiated by
     either fisetin or quercetin. However, the flavonoids
     potentiated epinephrine- or isoproterenol-induced lipolysis. Their effects were inhibited by propranolol (a .beta.-receptor antagonist).
     These results suggest that the flavonoids act synergistically with
     epinephrine on .beta.-adrenergic receptor and not through
     phosphodiesterase inhibition to stimulate adipocyte lipolysis. Increase
     in membrane phospholipid methylation occurred as a consequence of the
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epinephrine and/or quercetin/fisetin actions, and it correlated
     with the cellular accumulation of cAMP.
     Potentiation of .beta.-adrenoceptor agonist-mediated lipolysis
     by quercetin and fisetin in isolated rat adipocytes
     Quercetin and fisetin, two naturally occurring bioflavonoids mobilized
     lipids and enzymes in the absence or presence of epinephrine in intact rat
     adipocytes. Dose-(0-250 .mu.M) and time-(0-2 h) course studies, showed
     that they stimulated phosphodiesterase (PDE) activity and simultaneously
     exert cAMP accumulation. These bioflavonoids when present either singly
     or together with epinephrine stimulated the membrane-bound PDE but not the
     cytosolic PDE. The stimulation may act as a feedback mechanism to
     terminate the cAMP effects. The action of theophylline, a known
     lipolytic agent (exerting its effects through antagonism of
     adenosine Al receptor as well as PDE inhibition) was not potentiated by
     either fisetin or quercetin. However, the flavonoids
     potentiated epinephrine- or isoproterenol-induced lipolysis. Their
     effects were inhibited by propranolol (a .beta.-receptor antagonist).
     These results suggest that the flavonoids act synergistically with
     epinephrine on .beta.-adrenergic receptor and not through
     phosphodiesterase inhibition to stimulate adipocyte lipolysis.
     in membrane phospholipid methylation occurred as a consequence of the
     epinephrine and/or quercetin/fisetin actions, and it correlated
     with the cellular accumulation of cAMP.
     quercetin fisetin lipolysis epinephrine adipocyte;
     beta adrenergic receptor quercetin fisetin lipolysis
     Adipose tissue, metabolism
        (adipocyte, .beta.-adrenoceptor agonist-mediated lipolysis
        in, by quercetin and fisetin potentiation of)
     Adrenergic agonists
        (.beta.-, lipolysis from, quercetin and fisetin
        effect on, in adipocytes)
     Receptors
     RL: BIOL (Biological study)
        (.beta.-adrenergic, in epinephrine and quercetin and fisetin
        induction of lipolysis in adipocytes)
     51-43-4, Epinephrine 58-55-9, Theophylline, biological studies
     7683-59-2, Isoproterenol
     RL: BIOL (Biological study)
        (lipolysis from, quercetin and fisetin effect on,
        in adipocytes)
     60-92-4, Cyclic AMP
                           9025-82-5, Phosphodiesterase
     RL: BIOL (Biological study)
        (quercetin and fisetin effect on, in .beta.-adrenoceptor
        agonist-mediated lipolysis in adipocytes)
     117-39-5, Quercetin 528-48-3, Fisetin
     RL: BIOL (Biological study)
        (.beta.-adrenoceptor agonist-mediated lipolysis potentiation
        by, in adipocytes)
    ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER:
                        1992:625763 CAPLUS
DOCUMENT NUMBER:
                         117:225763
TITLE:
                        Effects of flavonoids on cyclic AMP phosphodiesterase
                         and lipid mobilization in rat adipocytes
AUTHOR (S):
                        Kuppusamy, U. R.; Das, N. P.
CORPORATE SOURCE:
                        Fac. Med., Natl. Univ. Singapore, Singapore, 0511,
                        Singapore
SOURCE:
                        Biochem. Pharmacol. (1992), 44(7), 1307-15
```

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal LANGUAGE: English

TI

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ΙT

IT

Thirty-one flavonoids were tested for their effects on low-Km AB phosphodiesterase (PDE) with cAMP as the substrate. Quercetin, luteolin, scutellarein, phloretin and genistein had inhibitory potencies comparable to or greater than that of 3-isobutyl-2-methylxanthine (EC50 30-50 .mu.M). Only 4 compds. (catechin, epicatechin, taxifolin and fustin) stimulated the enzyme activity (stimulatory EC50 130-240 .mu.M). The most potent PDE inhibitors were aglycons that had a C2,3 double bond, a keto group at C4 and hydroxyls at C3' and(or) C4'. However, when the C-ring is opened, the requirement for the C2,3 double bond is eliminated. The same series of flavonoids were also tested for their lipolytic activity. The structural features required for effective synergistic lipolysis (with epinephrine) were generally similar to those required for potent PDE inhibition, except that, for lipolytic activity, an intact C-ring was necessary. Fisetin and quercetin, having the above-mentioned structure, caused a concn. - and time-dependent increase in lipolysis which was synergistic with epinephrine. Only butein and hesperetin caused inhibition of epinephrine-induced lipolysis, and their effect was concn.-dependent. A time-course study indicated that hesperetin was able to delay the lipolytic action of epinephrine. It is most likely that the lipolytic effects of these compds. were not a result of PDE inhibition, as the orders of potency for the 2 activities had poor correlation. Apparently, the effectively lipolytic flavonoids were also potent PDE inhibitors but not all the PDE inhibitors were able to induce lipolysis. AB Thirty-one flavonoids were tested for their effects on low-Km phosphodiesterase (PDE) with cAMP as the substrate. Quercetin, luteolin, scutellarein, phloretin and genistein had inhibitory potencies comparable to or greater than that of 3-isobutyl-2-methylxanthine (EC50 30-50 .mu.M). Only 4 compds. (catechin, epicatechin, taxifolin and fustin) stimulated the enzyme activity (stimulatory EC50 130-240 .mu.M). The most potent PDE inhibitors were aglycons that had a C2,3 double bond, a keto group at C4 and hydroxyls at C3' and(or) C4'. However, when the C-ring is opened, the requirement for the C2,3 double bond is eliminated. The same series of flavonoids were also tested for their lipolytic activity. The structural features required for effective synergistic lipolysis (with epinephrine) were generally similar to those required for potent PDE inhibition, except that, for lipolytic activity, an intact C-ring was necessary. Fisetin and quercetin, having the above-mentioned structure, caused a concn. - and time-dependent increase in lipolysis which was synergistic with epinephrine. Only butein and hesperetin caused inhibition of epinephrine-induced lipolysis, and their effect was concn.-dependent. A time-course study indicated that hesperetin was able to delay the lipolytic action of epinephrine. It is most likely that the lipolytic effects of these compds. were not a result of PDE inhibition, as the orders of potency for the 2 activities had poor correlation. Apparently, the effectively lipolytic flavonoids were also potent PDE inhibitors but not all the PDE inhibitors were able to induce lipolysis. IT60-81-1, Phloridzin 60-82-2, Phloretin 90-19-7, Rhamnetin Chalcone 117-39-5, Quercetin 153-18-4, Rutin 154-23-4, Catechin 446-72-0, Genistein (flavan) 480-16-0, Morin 480-18-2, Taxifolin 480-40-0, Chrysin 480-41-1, Naringenin 486-66-8, Daidzein Flavanone 487-52-5, Butein 490-46-0, Epicatechin 491-70-3, Luteolin 520-18-3, Kaempferol 520-26-3, Hesperidin 520-27-4, Diosmin 520-34-3, Diosmetin 520-33-2, Hesperetin 520-36-5 525-82-6, Flavone 528-48-3, Fisetin 529-44-2, Myricetin 529-53-3, Scutellarein 5373-11-5, Luteolin-7-glucoside 10236-47-2 17912-87-7, 20725-03-5, Fustin Myricitrin RL: BIOL (Biological study) (cAMP phosphodiesterase inhibition by and lipolytic activity of, structure in relation to)

=> d ibib abs kwic 6-10

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:587368 CAPLUS

DOCUMENT NUMBER: 105:187368

TITLE: Effects of flavonoids on the production of volatile

sulfur compounds by anaerobes

AUTHOR(S): Hayashi, Hiroyuki

CORPORATE SOURCE: Oral Care Lab., Sun Star Co., Ltd., Takatsuki, 569,

Japan

SOURCE: Koku Eisei Gakkai Zasshi (1985), 35(4), 648-9

CODEN: KEGZA7; ISSN: 0023-2831

DOCUMENT TYPE: Journal LANGUAGE: Japanese

AB Morin, chrysin, and flavone in low concn. repressed the prodn. of volatile S compds. by oral anaerobes. The effect seems to be due to chem. or physiol. activity other than antibacterial activity. Myricetin, fisetin, and chalcone repressed the prodn. of volatile S compds. by their high antibacterial activity.

ΙT 94-41-7 480-16-0 480-40-0 525-82-6 **528-48-3** 529-44-2

RL: BIOL (Biological study)

(volatile sulfur compd. formation by oral anaerobes repression by)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1979:414915 CAPLUS

DOCUMENT NUMBER: 91:14915

TITLE: Inhibition of aflatoxin B1-induced cytotoxicity and

binding to DNA in cultured rat liver cells by

naturally occurring flavones

AUTHOR(S): Schwartz, Arthur G.; Rate, William R.

CORPORATE SOURCE:

Med. Sch., Temple Univ., Philadelphia, PA, 19140, USA

SOURCE: J. Environ. Pathol. Toxicol. (1979), 2(4), 1021-8

CODEN: JEPTDQ; ISSN: 0146-4779

DOCUMENT TYPE: Journal

LANGUAGE: English

GΙ

Four naturally occurring flavones, quercetin (I) AB[117-39-5], fisetin [528-48-3], nobiletin [478-01-3], and tangeretin [481-53-8], protected cultured rat liver epithelial-like cells against aflatoxin B1 (II) [1162-65-8]-induced cytotoxicity and inhibited the binding of II-3H to cellular DNA. The methoxy-substituted flavones, nobiletin and tangeretin showed greater protection against cytotoxicity than did the hydroxy-substituted compds., I and fisetin.

AΒ Four naturally occurring flavones, quercetin (I) [117-39-5], fisetin [528-48-3], nobiletin [478-01-3], and

tangeretin [481-53-8], protected cultured rat liver epithelial-like cells against aflatoxin B1 (II) [1162-65-8]-induced cytotoxicity and inhibited the binding of II-3H to cellular DNA. The methoxy-substituted flavones, nobiletin and tangeretin showed greater protection against cytotoxicity than did the hydroxy-substituted compds., I and fisetin.

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:123973 CAPLUS

DOCUMENT NUMBER: 74:123973

Investigation of flavones as fluorogenic spray TITLE:

reagents for organic compounds on a cellulose matrix.

II. Detection of pesticides Mallet, V.; Frei, Roland W.

AUTHOR(S): CORPORATE SOURCE: Dep. Chem., Dalhousie Univ., Halifax, Nova Scotia,

Can.

J. Chromatogr. (1971), 56(1), 69-77 SOURCE:

CODEN: JOCRAM

DOCUMENT TYPE: Journal LANGUAGE: English

Several classes of pesticides such as carbamates, s-triazines, organophosphates and chlorinated hydrocarbons were tested. Yellow fluorescent spots were obsd. on cellulose layers sprayed with fisetin. The visual detection limits obtained for these compds. with this new fluorogenic method range between 0.01 to 0.1 .mu.g. The method was also extended to herbicides and fungicides of a variety of chem. structures and conclusions were drawn as to the type of fluorescence phenomenon obsd. Some functional groups such as nitro and possibly amino, and mols. with a quinoid type of structure quenched the fluorescence of the spray reagent; while others, such as carboxylic, cyano and methoxy groups, did not.

AB Several classes of pesticides such as carbamates, s-triazines, organophosphates and chlorinated hydrocarbons were tested. Yellow fluorescent spots were obsd. on cellulose layers sprayed with fisetin. The visual detection limits obtained for these compds. with this new fluorogenic method range between 0.01 to 0.1 .mu.g. The method was also extended to herbicides and fungicides of a variety of chem. structures and conclusions were drawn as to the type of fluorescence phenomenon obsd. Some functional groups such as nitro and possibly amino, and mols. with a quinoid type of structure quenched the fluorescence of the spray reagent; while others, such as carboxylic, cyano and methoxy groups, did not.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1971:110750 CAPLUS

DOCUMENT NUMBER: 74:110750

TITLE:

Flavones as fluorogenic spray reagents for organic

compounds on a cellulose matrix. I. General

discussion of the method Mallet, V.; Frei, Roland W.

CORPORATE SOURCE: Dep. Chem., Dalhousie Univ., Halifax, NS, Can.

SOURCE: J. Chromatogr. (1971), 54(2), 251-7

CODEN: JOCRAM

DOCUMENT TYPE: Journal LANGUAGE: English

AUTHOR(S):

The usefulness of flavanol, fisetin, and robinetin (3-hydroxy-, 3,3',4',7-tetrahydroxy-, and 3,3',4',5',7-pentahy-droxyflavones, resp.), as fluorogenic spray reagents for polar org. compds. on cellulose thin-layer chromatograms was demonstrated by application to the pesticide Baygon (2-isopropoxyphenyl N-methylcarbamate). Spraying the chromatogram with 0.05% flavones in iso-PrOH and uv-irradn. gave intensely yellow pesticide spots on a slightly yellow background. The fluorescence was

sufficiently stable to permit possible applications in quant. pesticide anal. Apparently, the fluorescence is specific to 3-hydroxyflavones with an unsubstituted 5-position.

The usefulness of flavanol, **fisetin**, and robinetin (3-hydroxy-, 3,3',4',7-tetrahydroxy-, and 3,3',4',5',7-pentahy-droxyflavones, resp.), as fluorogenic spray reagents for polar org. compds. on **cellulose** thin-layer chromatograms was demonstrated by application to the pesticide Baygon (2-isopropoxyphenyl N-methylcarbamate). Spraying the chromatogram with 0.05% flavones in iso-PrOH and uv-irradn. gave intensely yellow pesticide spots on a slightly yellow background. The fluorescence was sufficiently stable to permit possible applications in quant. pesticide anal. Apparently, the fluorescence is specific to 3-hydroxyflavones with an unsubstituted 5-position.

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

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ORIGINAL REFERENCE NO.: 52:18383a-f

TITLE: Leucorobinetidin hydrate and leucofisetidin hydrate

AUTHOR(S): Roux, David G.; Freudenberg, Karl

CORPORATE SOURCE: Leather Ind. Research Inst., Grahamtown, S. Afr.

SOURCE: Ann. (1958), 613, 56-60

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

Unavailable cf. following abstr. Dihydrorobinetin, m. 226-8.degree., [.alpha.] 13.8.degree., was hydrogenated 6 hrs. in MeOH with PtO2, filtered, evapd., and taken up in H2O giving 3,3',4,4',5',7-hexahydroxyflavane dihydrate (I) (leucorobinetinidin hydrate), C15H14O7.2H2O, losing H2O at 70.degree. in vacuo, [.alpha.]D21 3.7.degree. (c 1, 50% Me2CO), turning red above 150.degree. and forming a viscous mass at 172-5.degree.. With CH2N2 at -5.degree., I in MeOH gave the 3',4',5',7-tetra-Me deriv. of I, C19H22O7 (II), m. 230-1.degree. (MeOH), a small amt. of which when heated 40 min. with 1 cc. 3N HCl and 3 cc. iso-PrOH gave a red, unanalyzed tetramethylanthocyanidin and another unidentified compd., sepd. chromatographically, which showed a brilliant yellow-green fluorescence. The 3,4-di-Ac deriv. of II (0.6 g.), m. 112-13.degree. (EtOH), was formed by heating II 5-7 min. with 5 cc. Ac2O and 1 g. AcONa. Treated similarly, I gave the hexa-Ac deriv. of I, m. 149-52.degree. (EtOH then MeOH). A mixt. of 3 g. 2,4-(HO)2C6H3CHO and 6 g. 3,4,5-(HO)3C6H2COCH2OH in 100 cc. anhyd. HCO2H was satd. with HCl at or below 0.degree., kept 16 hrs. at 20.degree., and poured into excess Et20 giving 1.63 g. 3,3',4',5',7-pentahydroxyflavylium chloride, C15H11ClO6 (robinetidin chloride) (III) thick, dark rhombs with green metallic luster (9:1 MeOH-concd. HCl), chromatographically homogeneous, giving a blue ppt. with AlCl3. I (a few mg.) in 4 cc. iso-PrOH and 1 cc. 3N HCl heated 2 hrs. at about 90.degree. gave III, identified by its Rf in various solvent systems and by the absorption max. of the Al complex, but contaminated with robinetin, as shown chromatographically. Rhus succedanea (or R. glabra) (1 kg.) wood meal was extd. repeatedly with hot AcOEt; the evapd. ext. in 500 cc. hot H2O on cooling gave a mixt. of fisetin (IV) and fustin (dihydrofisetin) (V), 5 g. of which in 200 cc. hot H2O was filtered through a Solka-floc cellulose column and developed with H2O; IV was retained as a yellow fluorescent zone and V formed a rapidly moving blue zone (colored by Fe) from which was isolated pure colorless V, m. 214-16.degree., [.alpha.]D21 -2.2.degree. (c 1.5, 50% Me2CO); tetraacetate, m. 150.degree.. V (2 g.) hydrogenated 8 hrs. in 50 cc. abs. EtOH with 0.4 g. PtO2, gave 3,3',4,4',7-pentahydroxyflavan (VI), C15H14O6.0.5 H2O sintering 110.degree., decomp. about 126-30.degree. (after drying-over P205 in vacuo), [.alpha.]D21 -2.4.degree. (c 1.4, 50% Me2CO). VI in MeOH at -5.degree. with CH2N2 gave the 3',4',7-trimethyl deriv. (VII), rosettes, m. 150-1.degree. or fine needles, sintering

68-70.degree., m. 149.degree. (EtOH or iso-Pr20), [.alpha.]D21 0.5.degree. [c 1.05, 2:1 (CHCl)2MeOH]. The 3,4-di-Ac deriv. of VII m. 121-2.degree. (EtOH). The penta-Ac deriv. of VI, noncryst. granules, giving satisfactory analytical data, was formed from VI with pyridine and Ac20. Without giving details, R. and F. allude to the leucofisetinidin hydrate, obtained from quebracho wood, (cf. following abstract). cf. following abstr. Dihydrorobinetin, m. 226-8.degree., [.alpha.] AB 13.8.degree., was hydrogenated 6 hrs. in MeOH with PtO2, filtered, evapd., and taken up in H2O giving 3,3',4,4',5',7-hexahydroxyflavane dihydrate (I) (leucorobinetinidin hydrate), C15H14O7.2H2O, losing H2O at 70.degree. in vacuo, [.alpha.]D21 3.7.degree. (c 1, 50% Me2CO), turning red above 150.degree. and forming a viscous mass at 172-5.degree.. With CH2N2 at -5.degree., I in MeOH gave the 3',4',5',7-tetra-Me deriv. of I, C19H22O7 (II), m. 230-1.degree. (MeOH), a small amt. of which when heated 40 min. with 1 cc. 3N HCl and 3 cc. iso-PrOH gave a red, unanalyzed tetramethylanthocyanidin and another unidentified compd., sepd. chromatographically, which showed a brilliant yellow-green fluorescence. The 3,4-di-Ac deriv. of II (0.6 g.), m. 112-13.degree. (EtOH), was formed by heating II 5-7 min. with 5 cc. Ac20 and 1 g. AcONa. Treated similarly, I gave the hexa-Ac deriv. of I, m. 149-52.degree. (EtOH then MeOH). A mixt. of 3 g. 2,4-(HO)2C6H3CHO and 6 g. 3,4,5-(HO)3C6H2COCH2OH in 100 cc. anhyd. HCO2H was satd. with HCl at or below 0.degree., kept 16 hrs. at 20.degree., and poured into excess Et20 giving 1.63 g. 3,3',4',5',7-pentahydroxyflavylium chloride, C15H11Cl06 (robinetidin chloride) (III) thick, dark rhombs with green metallic luster (9:1 MeOH-concd. HCl), chromatographically homogeneous, giving a blue ppt. with AlCl3. I (a few mg.) in 4 cc. iso-PrOH and 1 cc. 3N HCl heated 2 hrs. at about 90.degree. gave III, identified by its Rf in various solvent systems and by the absorption max. of the Al complex, but contaminated with robinetin, as shown chromatographically. Rhus succedanea (or R. glabra) (1 kg.) wood meal was extd. repeatedly with hot AcOEt; the evapd. ext. in 500 cc. hot H2O on cooling gave a mixt. of fisetin (IV) and fustin (dihydrofisetin) (V), 5 g. of which in 200 cc. hot H2O was filtered through a Solka-floc cellulose column and developed with H2O; IV was retained as a yellow fluorescent zone and V formed a rapidly moving blue zone (colored by Fe) from which was isolated pure colorless V, m. 214-16.degree., [.alpha.]D21 -2.2.degree. (c 1.5, 50% Me2CO); tetraacetate, m. 150.degree.. V (2 g.) hydrogenated 8 hrs. in 50 cc. abs. EtOH with 0.4 g. PtO2, gave 3,3',4,4',7-pentahydroxyflavan (VI), C15H14O6.0.5 H2O sintering 110.degree., decomp. about 126-30.degree. (after drying-over P205 in vacuo), [.alpha.]D21 -2.4.degree. (c 1.4, 50% Me2CO). VI in MeOH at -5.degree. with CH2N2 gave the 3',4',7-trimethyl deriv. (VII), rosettes, m. 150-1.degree. or fine needles, sintering 68-70.degree., m. 149.degree. (EtOH or iso-Pr20), [.alpha.]D21 0.5.degree. [c 1.05, 2:1 (CHCl) 2MeOH]. The 3,4-di-Ac deriv. of VII m. 121-2.degree. The penta-Ac deriv. of VI, noncryst. granules, giving satisfactory analytical data, was formed from VI with pyridine and Ac20. Without giving details, R. and F. allude to the leucofisetinidin hydrate, obtained from quebracho wood, (cf. following abstract).

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